Thermopower of Kondo Effect in Single Quantum Dot Systems with Orbital at Finite Temperatures

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Abstract

We investigate the thermopower due to the orbital Kondo effect in a single quantum dot system by means of the noncrossing approximation. It is elucidated how the asymmetry of tunneling resonance due to the orbital Kondo effect affects the thermopower under gate-voltage and magnetic-field control.

1. Introduction

The Kondo effect due to magnetic impurity scattering in metals is a well known and widely studied phenomenon [1]. The effect has recently received much renewed attention since it was found that the Kondo effect significantly influences the conductance in quantum dot (QD) systems [2]. A lot of tunable parameters in QD systems have made it possible to systematically investigate electron correlations. In particular, high symmetry in shape of QDs gives rise to the orbital properties, which has stimulated extensive studies on the conductance due to the orbital Kondo effect [3,4,5,6,7,8]. The thermopower we study in this paper is another important transport quantity, which gives complementary information on the density of states to the conductance measurement: the thermopower can sensitively probe the asymmetric nature of the

tunneling resonance around the Fermi level. So far, a few theoretical studies have been done on the thermopower in QD systems [9,10,11,12,13,14,15,16]. A recent observation of the thermopower due to the spin Kondo effect in a lateral QD system [17] naturally motivates us to theoretically explore this transport quantity in more detail. Here, we discuss how the asymmetry of tunneling resonance due to the orbital Kondo effect affects the thermopower under gate-voltage and magnetic-field control. By employing the noncrossing approximation (NCA) for the Anderson model with finite Coulomb repulsion, we especially investigate the Kondo effect of QD for several electron-charge regions.

2. Model and Calculation

Let us consider a single QD system with N-degenerate orbitals in equilibrium, as shown in Fig. 1. The energy levels of the QD are assumed to be

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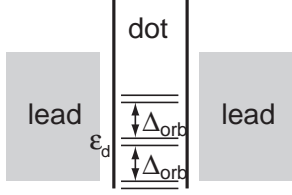[1] E-mail: sakano@tp.ap.eng.osaka-u.ac.jp

Fig. 1. Energy-level scheme of a single QD system with three orbitals coupled to two leads.

$$\varepsilon_{\sigma l} = \varepsilon_d + l\Delta_{orb}, \tag{1}$$

$$l = -(N_{orb} - 1)/2, -(N_{orb} - 3)/2, \cdots, (N_{orb} - 1)/2$$

where ε_d denotes the center of the energy levels and σ (l) represents spin (orbital) index and N_{orb} represents the degree of the orbital degeneracy. The energy-level splitting between the orbitals Δ_{orb} is induced in the presence of magnetic field B; $\Delta_{orb} \propto B$. In addition, the Zeeman splitting is assumed to be much smaller than the orbital splitting, so that we can ignore the Zeeman effect. In practice, this type of orbital splitting has been experimentally realized as Fock-Darwin states in vertical QD systems or clockwise and counter-clockwise states in carbon nanotube QD systems. Our QD system is described by the multiorbital Anderson impurity model,

$$\mathcal{H} = \mathcal{H}_l + \mathcal{H}_d + \mathcal{H}_t \tag{2}$$

$$\mathcal{H}_l = \sum_{k\sigma l} \varepsilon_{k\sigma l} c^\dagger_{k\sigma l} c_{k\sigma l}, \tag{3}$$

$$\mathcal{H}_d = \sum_{k\sigma l} \varepsilon_{\sigma l} d^\dagger_{\sigma l} d_{\sigma l} + U \sum_{\sigma l \neq \sigma' l'} n_{\sigma l} n_{\sigma' l'}$$

$$\qquad - J \sum_{l \neq l'} \boldsymbol{S}_{dl} \cdot \boldsymbol{S}_{dl'}, \tag{4}$$

$$\mathcal{H}_t = V \sum_{k\sigma} \left(c^\dagger_{k\sigma l} d_{\sigma l} + \text{H. c.} \right), \tag{5}$$

where U is the Coulomb repulsion and $J(> 0)$ represents the Hund coupling in the QD.

The non-equilibrium Green's function technique allows us to study general transport properties, which gives the expression for the T-linear thermopower as [14],

$$S = -(1/eT)(\mathcal{L}_{12}/\mathcal{L}_{11}), \tag{6}$$

with the linear response coefficients,

$$\mathcal{L}_{11} = \frac{\pi T}{h} \Gamma \sum_{\sigma l} \int d\varepsilon\, \rho_{\sigma l}(\varepsilon) \left(-\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right), \tag{7}$$

$$\mathcal{L}_{12} = \frac{\pi T}{h} \Gamma \sum_{\sigma l} \int d\varepsilon\, \varepsilon \rho_{\sigma l}(\varepsilon) \left(-\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right), \tag{8}$$

where $\rho_{\sigma l}(\varepsilon)$ is the density of states for the electrons with spin σ and orbital l in the QD and $f(\varepsilon)$ is the Fermi distribution function. In order to obtain the thermopower it is necessary to evaluate $\rho_{\sigma l}(\varepsilon)$.

We exploit the NCA method to treat the Hamiltonian (2) [18,19]. The NCA is a self-consistent perturbation theory, which summarizes a specific series of expansions in the hybridization V. This method is known to give physically sensible results at temperatures around or higher than the Kondo temperature. The NCA basic equations can be obtained in terms of coupled equations for the self-energies $\Sigma_m(z)$ of the resolvents $R_m(z) = 1/[z - \varepsilon_m - \Sigma_m(z)]$,

$$\Sigma_m(z) = \frac{\Gamma}{\pi} \sum_{m'} \sum_{\sigma l} \left[\left(M^{\sigma l}_{m'm} \right)^2 + \left(M^{\sigma l}_{mm'} \right)^2 \right]$$

$$\qquad \times \int d\varepsilon R_{m'}(z + \varepsilon) f(\varepsilon), \tag{9}$$

where the index m specifies the eigenstates of $\mathcal{H}_d$ and the mixing width is $\Gamma = \pi \rho_c V^2$. The coefficients $M^{\sigma l}_{mm'}$ are determined by the expansion coefficients of the Fermion operator $d^\dagger_{\sigma l} = \sum_{mm'} M^{\sigma l}_{mm'} |m\rangle\langle m'|$. We compute the density of states by this method to investigate the thermopower.

3. Results

3.1. Gate voltage control

The thermopower for two orbitals is shown in Fig. 2 as a function of the energy level ε_d (gate-voltage control). There are four Coulomb peaks around $-\varepsilon_d/U \sim 0, 1, 2, 3$ at high temperatures (see the inset of Fig. 2(a)). As the temperature decreases, the thermopower in the region of $-1 < \varepsilon_d/U < 0 (-3 < \varepsilon_d/U < -2)$ with $n_d \sim 1(3)$ is dominated by the $SU(4)$ Kondo effect. The thermopower has negative values in the region $-1 < \varepsilon_d/U < 0$, implying that the effective tunneling resonance, such as the Kondo resonance, is located above the Fermi level. At low enough temperatures, the $SU(4)$ Kondo effect is enhanced with decrease of en-
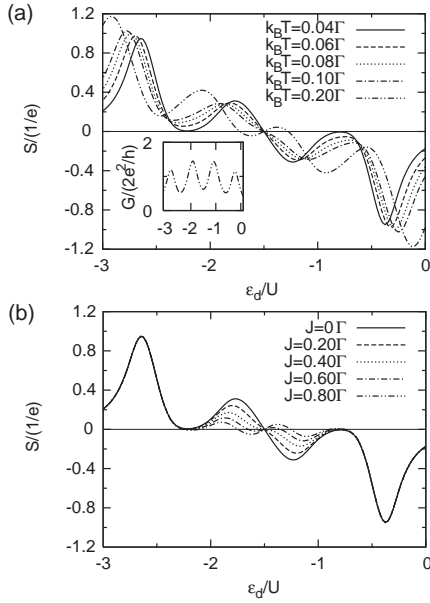
Fig. 2. The thermopower for the two orbital QD system with finite Coulomb repulsion $U = 8\Gamma$ as a function of the energy level of the QD. (a) The temperature dependence for $J = 0$. The inset shows the conductance as a function of the dot level at $k_B T = 0.20\Gamma$ (Coulomb resonance peaks). (b) The Hund-coupling dependence for $k_B T = 0.04\Gamma$.
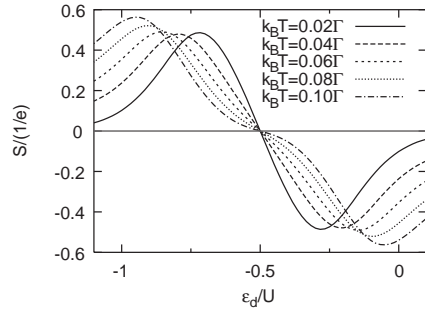

Fig. 3. The thermopower due to the ordinary spin Kondo effect as a function of the dot level. We set $U = 6\Gamma$.
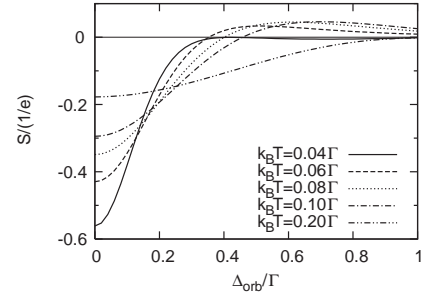

Fig. 4. The thermopower for the two orbital QD system, in case of $\varepsilon_d = -U/2$, as a function of orbital splitting Δ_{orb}. We set $U = 8\Gamma$.

ergy level down to $\varepsilon_d/U = -1/2$, which results in the enhancement of the thermopower. However, if the temperature of the system is larger than the $SU(4)$ Kondo temperature, the Kondo effect is suppressed and the thermopower has a minimum in the regime $-1/2 < \varepsilon_d/U < 0$. As the energy level further decreases, the $SU(4)$ Kondo effect and the resulting thermopower are both suppressed. Note that the Hund coupling hardly affects the thermopower because of $n_d \sim 1$ in this regime, as shown in Fig. 2 (b). Since the region of $-3 < \varepsilon_d/U < -2$ can be related to $-1 < \varepsilon_d/U < 0$ via an electron-hole transformation, we can directly apply the above discussions on the $SU(4)$ Kondo effect to the former region by changing the sign of the thermopower.

Let us now turn to the region of $-2 < \varepsilon_d/U < -1$, where $n_d \sim 2$. At $J = 0$, the Kondo effect due to six-fold degenerate states occurs. Although the resulting Kondo effect is strongly enhanced around $\varepsilon_d/U = -3/2$ in this case, the thermopower is almost zero because the Kondo resonance is located just at the Fermi level. Therefore, when the dot level is changed, the position of the Kondo resonance is shifted across the Fermi

level, which causes the sign change of the thermopower. Around $\varepsilon_d/U = -3/2$, even small perturbations could easily change the sign of the thermopower at low temperatures. Note that these properties are quite similar to those for the ordinary spin Kondo effect shown in Fig. 3, because the filling is near half in both cases. For large Hund couplings J, the triplet Kondo effect is realized and the resulting Kondo temperature is very small, so that the thermopower shown in Fig. 2(b) is dramatically suppressed.

3.2. Magnetic field control

Let us now analyze the effects of orbital-splitting caused by magnetic fields. The computed thermopower for $\varepsilon_d/U = -1/2$ is shown in Fig. 4 as a function of the orbital splitting Δ_{orb}. It is seen that magnetic fields dramatically suppress the thermopower, which is caused by the following mechanism. In the presence of magnetic fields, the Kondo effect changes from the $SU(4)$ orbital type to the $SU(2)$ spin type because the orbital degeneracy is lifted. As a consequence, the res-

onance peak approaches the Fermi level and the effective Kondo temperature is reduced, so that the thermopower at finite temperatures is reduced in the presence of magnetic fields.

Note that, in our model, magnetic fields change the lowest energy level $\varepsilon_{\sigma-\frac{1}{2}}$ from $-U/2$ to $-(U+\Delta_{orb})/2$. Accordingly, the peak position of the renormalized resonance shifts downward across the Fermi level (down to a little below the Fermi level). Thus, the large negative thermopower changes to a small positive one as the magnetic field increases at low temperatures. In strong fields, the effective Kondo resonance is located around the Fermi level with symmetric shape, so that even small perturbations could give rise to a large value of thermopower with either negative or positive sign.

Finally a brief comment is in order for other choices of the parameters. The thermopower for $\varepsilon_d/U = -5/2$ shows similar magnetic-field dependence to the $\varepsilon_d/U = -1/2$ case except that its sign is changed. For $\varepsilon_d/U = -3/2$, the thermopower is almost zero and independent of magnetic fields, because the Kondo resonance is pinned at the Fermi level and gradually disappears with increase of magnetic fields.

4. Summary

We have studied the thermopower for the two-orbital QD system under gate-voltage and magnetic-field control. In particular, making use of the NCA method for the Anderson model with finite Coulomb repulsion, we have systematically investigated the low-temperature properties for several electron-charge regions. It has been elucidated how the asymmetric nature of the resonance due to the orbital Kondo effect controls the magnitude and the sign of the thermopower at low temperatures.

For $\varepsilon_d/U \sim -1/2$ ($\varepsilon_d/U \sim -5/2$), where $n_d \sim 1(3)$, the $SU(4)$ Kondo effect is dominant and the corresponding thermopower is enhanced. These two regions are related to each other via an electron-hole transformation, which gives rise to an opposite sign of the thermopower. In addition, magnetic fields change the Kondo effect to an $SU(2)$ type, resulting in two major effects: the effective resonance position approaches the Fermi level and the Kondo temperature is decreased. Therefore, the reduction of the thermopower occurs in the presence of magnetic fields.

For $\varepsilon_d/U \sim -3/2$, where $n_d \sim 2$, the Kondo effect due to six-fold degenerate states occurs for $J = 0$. However, the thermopower is strongly reduced because the resonance peak is located near the Fermi level. When the Hund coupling is large, the triplet Kondo effect is dominant. The resulting small Kondo temperature suppresses the thermopower around $\varepsilon_d/U \sim -3/2$ at finite temperatures. In this region, magnetic fields do not affect the asymmetry of the resonance peak and the resulting thermopower remains almost zero because the filling is fixed.

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